

**Dienstag, 12.05.2015**

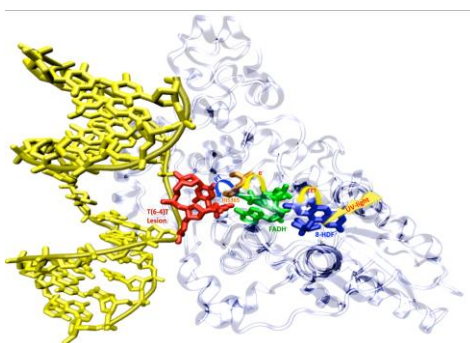
**Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

**Sprecher: Shirin Faraji**  
(Universität Heidelberg)

**Titel: Utilizing light for repair of light-induced  
DNA damages: the clever mode of action  
of DNA photolyases**

### **Abstract:**

When DNA is exposed to far-UV radiation, radiant energy triggers various chemical reactions such as intra-strand cross-linking between adjacent pyrimidines causing genetic mutations. DNA photolyases are enzymes initiating cleavage of mutagenic pyrimidine (6-4) pyrimidine photolesions by a photoinitiated electron transfer from flavin adenine dinucleotide to the lesion.



Using state-of-the-art hybrid quantum mechanical/molecular mechanical (QM/MM) dynamics, we have carried out a series of simulations to completely map out the entire evolution of functional processes to reveal the molecular mechanism of this important biological function. We have demonstrated that the electron catalysing the repair is generated via an intermolecular coulombic decay (ICD) process [1]. In fact, this is the first example for ICD as operating mechanism in a real biological system. The electron-induced repair mechanism occurs in the electronic ground state of the lesion radical anion. In sum, we have presented the first energetically feasible molecular repair mechanism in which the initial step is electron transfer coupled to proton transfer from the protonated Histidine to the lesion [2]. This makes the formation of an oxetane-like transition state possible, along which OH group is transferred to 3-primidone. This newly identified pathway requires neither a two-photon process nor electronic excitation of the photolesion. Our theoretical findings are in agreement with experimental time resolved findings and for the first time the experimental spectroscopic signature of the detected (6-4) intermediate is assigned theoretically to a specific molecular structure [3].

1. P. Harbach, M. Schneider, S. Faraji, A. Dreuw, *J. Phys. Chem. Lett.* 4, 943 (2013).
2. a) S. Faraji, G. Groenhof and A. Dreuw, *J. Phys. Chem. B.* 117, 10071 (2013), b) S. Faraji and A. Dreuw, *Ann. Rev. Phys. Chem.* 64, (2014).
3. a) J. Li et al, *Nature* 466, 887 (2010). b) S. Faraji, D. Zohng, and A. Dreuw, *Angew. Chem. Int. Ed.* Revision step (2015).

**Organisation: B. Engels**

**Kontakt:** Prof. Dr. Roland Mitric, Institut für Physikalische und Theoretische Chemie,  
[roland.mitric@uni-wuerzburg.de](mailto:roland.mitric@uni-wuerzburg.de)  
Weitere Informationen unter:  
<http://www.phys-chemie.uni-wuerzburg.de/startseite/veranstaltungen/>